Level 2 Product v2.1 (007-08-0310) Release Notes

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We request that the version 2.1 data (hereafter refered to as "v2.1") should be used very cautiously for scientific purposes, under the condition that you know characteristics of the data well. This product will be released to the general users (not limited within SMILES RA researchers) soon.

Brief overview of improvement in v2.1:

Precision of HOCl product has been improved. In addition, several line parameters have been updated. See Section 5 for the details of these updates. For the details of data format, please refer to "JEM/SMILES L2 Product Guide for Ver.2.1 (007-08-0310)".

1. SMILES observation

- SMILES observes 624-650 GHz in three bands defined as bands A, B, and C. Since the SMILES instrument consists of two receivers, emission in band A can be measured by different receivers according to the combination of observed bands.
- The period of coverage is from October 12, 2009 to April 21, 2010.
  - From November 30 to December 15, 2009, the ISS solar paddle stopped just in front of the SMILES IFOV due to the maintenance of the Port Solar Alpha Rotary Joint elements of the ISS.
  - From February 25 to March 5, 2010, the number of L1B data is only around 10% of ordinary condition, due to trouble of communication system of ISS/JEM (not according to SMILES itself).

2. Two types of L2 Products

- There are two types of products.
  - *L2Product_G_RA* (0.8 MB/file, 1 file/day/molecule)
    - This product has minimum information such as retrieved profiles, precisions and a simple status flag.
    - The profile data derived from single observation band are contained in the product, according to the priority (see Table 1) and the number of available profiles day by day. Therefore, it should be noted that the observation band may not be continuous, though the data series itself continuous.
  - *L2Product* (8MB/file, 1 file/day/molecule/band)

- ✧ This product has detailed information, such as a detailed status flag, a priori profiles and averaging kernels. Refer to the Product Guide for details.
- ✧ The profile data derived from all observation bands are contained in this product.

Table 1 standard products and ban priority

Product	Priority	Product	Priority	Product	Priority
O_3	A, B(, C)	HCl	B, A	ClO	C
HNO_3	C(, A)	HOCl	A	CH_3CN	A
BrO	C(, A)	HO_2	B, C	Temperature	A, B
^{17}OOO	C	$O^{17}OO$	B	^{18}OOO	B, C

3. Data screening for scan

- This version of the L2 product includes all the processed profiles, so some of them are inadequate for scientific use. In using these profiles, it is strongly recommended to pick up usable ones according to the following screening conditions (see Table 2, Figure 1, and Figure 2); also please look at 4. Data screening for Altitude as to the usable altitude range for each species.
  - ➢ Quick method: Users check only a *Status* field and can reject inadequate scans.
    - ✧ A *Status* field has a value 0 only in case that all of FOV interference, observation altitude range, and convergence status are qualified (see Table 3). This criterion gives priority to the data quality over the number of available data, therefore about 30 to 60% (depend on the observation band) of scan data will be removed
  - ➢ Advanced methods: Users check individual fields that show error status.
    - ✧ The 1st bit of *Status* field shows the error flag of FOV interference. When the interference is predicted (the *FOVInterference* field > 0) or forecast information is lost (*FOVInterference* = -1), this flag is set. (see Table 4) . About 20% of the profile data will be removed with this criterion. However, this constraint is very "conservative", therefore about 70% of removed data may be adequate to use. If you want to utilize as more data as possible, you may ignore this flag.
    - ✧ The 2nd bit shows the error flag of observation altitude range. You may not ignore this flag.
    - ✧ The 3rd bit shows the error flag of convergence of the retrieval process.

When the convergence is not well (the *Convergence* field > 1), this flag is set. However, in case of the species which has strong spectral line (such as O_3, HCl, and ClO), you may ignore this flag and apply "looser" constraint such as *Convergence* < 10, because the retrieved profiles of those species are relatively good even the retrieval process was not well converged. Especially in case of band C, if you apply the constraint *Convergence* < 10, you can obtain 30% more available data than those by the screening result with this flag.

Table 2 Samples of screening condition

	Useful condition	Usable products type	Useful data(%)		
			A	B	C
Quick	Status = 0	L2Product L2Product_G_RA	68	59	38
Advanced 1 (except for O_3, HCl, ClO)	*Convergence* = 1 or 3rd bit of *Status* = 0 2nd bit of *Status* = 0	L2Product L2Product_G_RA	83	75	45
Advanced 2 (for O_3, HCl, ClO)	*Convergence* < 10 2nd bit of *Status* = 0	L2Product only	92	90	72

Table 3 *Status* field

Value	Explanation
0	No error status
>0	ERROR status, Do not use this profiles
1	FOV interference error (*FOVInterference* ≠ 0)
2	Observation altitude error
4	Convergence status error (*Convegences* > 1)

Table 4 *FOVInterference* field

Value	Explanation
-1	No interference forecast information
0	No FOV interference
>0	Do not use this profile
1	Information: FOV interference by Sun
2	Information: FOV interference by Moon
4	Information: FOV interference by ISS Solar paddle

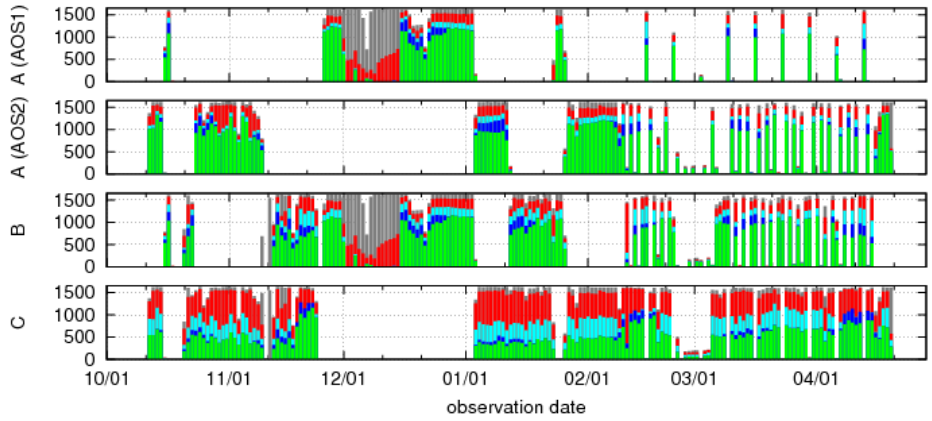

Figure 1: The number of screened scan data. Green: screened with "Quick" condition, Blue: additionally screened with "Advance1" condition, Light blue: additionally screened with "Advance2" condition, Red: without any conditions, Gray: not contained within L2 products.

(Note: These figures are drawn with v2.0 data, because they will be same as the results from v2.1.)

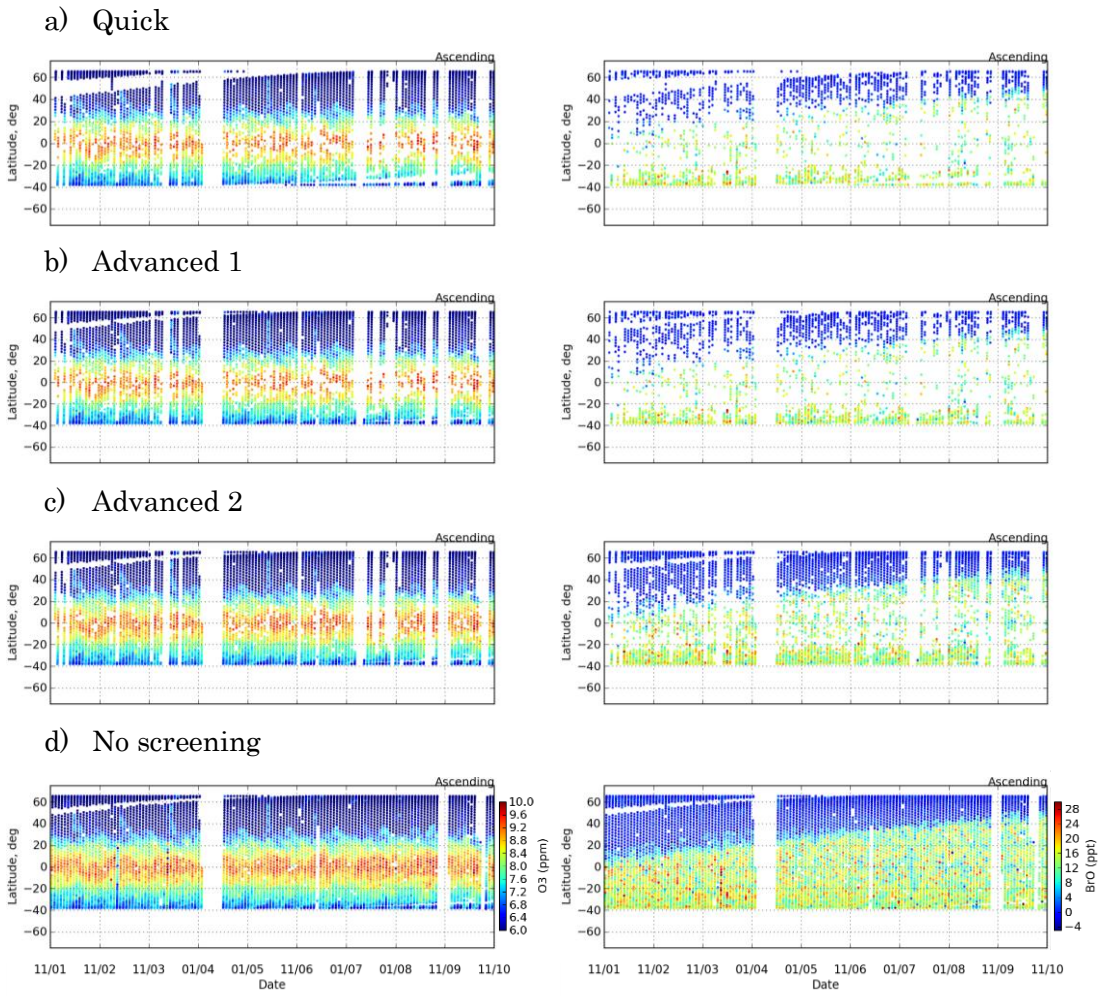

Figure 2: Examples of screening results projected on the latitude-time cross-section. Observation data from November 1 to 10, 2009, at the altitude of 28km (only from ascending orbits). Left: O_3, from Band A,. Right: BrO, from Band C.

(Note: These figures are drawn with v2.0 data, with the same reason as Figure 1.)

4. Data screening for Altitude

- The L2 products include data for altitude range not usable to validation and/or science. If the *L2Precision* is more than 50% compared to the *AprioriError*, it is probable that L2 algorithm is just answering *a priori*. In this case, the value of *L2Precision* was turned into negative. (*L2Precision* and *AprioriError* are defined as HDF EOS5 names in the SMILES L2 products.)

5. Improvements in v2.1 updates

- The HOCl product was improved in this version. Other products such as O_3 have not been changed.
- Some line parameters have been updated (see Table 5). HOCl spectral lines are located at the shoulder of these lines. Residual spectra around HOCl were suppressed.

Table 5 updated line parameters

Parameters	L2 v2.0	v2.1	Reference
$O_{3(v1,3)}$ (625012.89 MHz)			
- **γ_0 (MHz/hPa)**	2.3078	2.017	HITRAN 2008
- n_γ	0.78	0.76	
$O_{3(v1,3)}$ (625051.27 MHz)			
- **γ_0 (MHz/hPa)**	2.3078	2.172	
- n_γ	0.78	0.79	
^{18}OOO			
- **Line position (MHz)**	625088.260 625091.258	625090.4623 625091.8080	JPL catalog

6. Newly Found Issue in v2.1

- There is no problem found according to update from v2.0 to v2.1.

7. Remaining Issues

- HOCl, HNO_3 (in band A) and BrO data (in band A) look not usable. [Continuing from v1.0]
- We recommend zonal mean processing on using CH_3CN, BrO (in band C), HNO_3 (in band C) and HO_2 data.
- Checking of O_3 isotope products have not been sufficiently done yet. [Continuing from v1.0]
- According to the change of retrieval altitude grid, altitude grids of the species in

single product are not uniform. In the future, we consider to apply the pressure grids uniformly among the species. In addition, we are studying some improvements of L2 retrieval algorithm. [Continuing from v1.3]

- Convergence state in band C is not good. Only 40 – 50% of scans satisfy convergence condition, while 70-80% of scans satisfy in case of band A and B. We try to improve this by taking into account results from Band A or B. [Continuing from v2.0]
- Dicke narrowing effect was not considered and the profiles in upper mesosphere may have negative bias. However, we have found this effect is actually small. [Continuing from v2.0]
- Zeeman splitting is not implemented to ClO, BrO, and HO_2 in forward model calculation, which may affect these products above 60km. [Continuing from v2.0]
- Frequency calibration in the L1 processing has a long-term drift. [Continuing from v2.0]

References

Ochiai, S., Kikuchi, K., Nishibori, T., Mizobuchi, S., Manabe, T., Mitsuda, C., and Baron, P., 2011, "Gain nonlinearity calibration of the SMILES receiver," IEEE International Geoscience and Remote Sensing Symposium, Vancouver, 3610

Ozeki, H., Tamaki. K., Mizobuchi, S., Mitsuda, C., Sano, T., Suzuki. M., Kikuchi, K., and Shiotani, M., 2011, "Response characteristics of radio spectrometers of the Superconducting Submillimeter-Wave Limb-Emission Sounder (JEM/SMILES)," IEEE International Geoscience and Remote Sensing Symposium, Vancouver, 3619

Appendixes - Information in the previous versions

- Description in v1.0
  - The tangent altitude (geometrical) is calculated by using a) SMILES Star Sensors, b) SMILES scan mirror angle, and c) ISS position. SMILES star sensor shows unexpected large scattered output. We smoothed out the SMILES tangent altitude by second order fitting in this version. The tangent altitude precision should be 100 m (1 sigma) in rms by the specification, which is now under verification.
  - The two SMILES star sensors are pointing somewhat close direction each other, thus there is possibility that the SMILES tangent point cannot be calculated when both the sensors are within 45° to the Sun. In this situation, no L2 product is processed.
  - The tangent altitude for L2 data is retrieved as an altitude offset.
  - Condition of vertical correlation is not introduced in the retrieval of all species except temperature, according to the result of vertical correlation study.

- Improvements at v1.1 update
  - The pointing direction for determining tangent altitudes (geometrical) is calculated by using SMILES scan mirror angle and ISS position. However, since the pointing accuracy heavily would affect to error of tangent altitude determination, an average altitude within single scan is retrieved with using the Star Sensor of SMILES in L2 processing. In case that sunlight or moonbeam enters in the FOV of SMILES Star Sensor, positioning information cannot be obtained, so it will be estimated from the information of 50 scans around the scan in such cases.

- Improvements at v1.2 update
  - Illegal value in longitude in case the longitude of tangent point is around 180 degree, has been corrected.
  - Altitude offset of Star Trackers (STT) has been reduced to +/- 1km, according to implementation of compensation formula of time from STT.
  - Rate of convergence in the retrieval process has been improved, by smoothing vibrations in the ISS altitude data which do not seem to represent actual vibrations.
  - Description of line shape has been refined with introducing the coefficient

(ν/ν_0).

- Line parameters of O_3, HNO_3, HO_2 and ozone isotopes have been changed from the JPL catalog to HITRAN2008.
- Profiles of temperature and HCl around 50km have been improved, with compensation of an effect from the Doppler shift.
- Consistency between retrieval results from band A in Setting 2 (band A/C) and Setting 3 (band B/A) have been improved, by taking compensation between the response function of AU1 and AU2 (2 units in AOS).
- Hydrostatic assumption has been introduced as a constraint in the calculation of pressure and temperature.
- Retrieval results of HOCl have been improved, by ignoring ozone isotopes whose absorption lines overlap that of HOCl in band A.
- Information contents of ozone isotopes, HNO3, ClO and CH_3CN have been increased, by adjusting the error value in *a priori* profile.
- Rate of convergence in the retrieval process has been increased, by ignoring temperature retrieval in band C.
- Rate of convergence in the retrieval process has been increased, by raising upper limit of iteration trials in the retrieval process from 5 to 8.

- Improvements at v1.3 update
  - L1B data have been updated from version 005 to 006. The retrieved profiles from the scans near "FOV interference" were improved by referring "the flags indicating FOV disturbance." For details of L1B data update, see the document "Level 1 Product Release Notes (Ver.006)".
  - Standard temperatures for Lorentz width of absorption lines of O_3, HNO_3, HO_2 and ozone isotopes have been corrected from 300K to 296K. The effect for this correction is around a few percent.
  - In correcting the tangent height on the observation point, it is introduced that the antenna elevation offset is retrieved from the average of altitude offset within one scan. According to this change, O_3 and HCl above 50km increase a few percent.
  - Antenna movement within the time to acquire a spectrum for single height is taken into account with the antenna pattern. This improvement causes a few percent increase of ozone at the peak height (lower stratosphere).
  - In order to make better fitting of the curved baseline of brightness temperature, the uncertainty of absorption coefficient is fitted with 2-dimensional function

instead of 1-dimensional. As a result, residue of the baseline has been decreased to about a half in comparison with the previous version.

- Regularization of status vectors in the inversion model with a priori error have been introduced. According to this improvement, 2-dimensional term of the absorption coefficients with small number of digits can be retrieved.
- The grids of retrieval altitude have been adjusted 2, 3 or 4 km depending on species, band and altitude, instead of uniformly 3km in the previous version. In adjusting the altitude grid, the information of altitude resolution is referred. As a result of this modification, the species with high sensitivity (such as O_3 and HCl) can be retrieved with more precise altitude grid, and the one with low sensitivity (such as BrO and HO_2) can be retrieved with wider altitude range.
- The altitude correlation of 10km has been introduced for all products except O_3 from band A and B.
- The information of convergence, FOV interference and observation altitude are stored in the *status* field. For details, see the format sheet in the Product Guide of v1.3.
- In order to evaluate the residue of spectrum, the cost function for all species and all altitudes are stored in the *CostFunctionY* and *CostFunctionYAll* fields in the products.
- Bugs in the *AveragingKernel*, *InformationValue* and *VerticalResolution* fields have been fixed.
- Preliminary "status flag" has been newly added from this versionFor the retrieval of Band C, a priori value of the tangent altitude is provided from Band A or B. (There are operational modes with Band A+C and Band B+C.)

- Improvements in v2.0 updates
  - L1B data have been updated from version 006 to 007.
    - ✧ Gain nonlinearity correction has been applied to observed spectra (Ochiai *et al.*, 2011). In the middle stratosphere, retrieved temperatures become closer to those of Goddard Earth Observing System-5 assimilated data. Nonlinearity effects influence not only temperature but also other molecules. For those species such as O_3, HCl and ClO with strong lines the retrieved values decrease by 5 – 7% in 25 – 45 km. For those species such as HOCl and BrO with weak lines located at the wing of strong lines the retrieved values change about 50 – 100 %. In v1.3, the retrieved profiles of HOCl contained negative values around 30km, but it is now improved.

- New AOS response function has been introduced. This function is modeled by new on-orbit measurement data for AOS response function in January of 2011 (Ozeki *et al.*, 2011).
- Temperature field in the mesosphere is very sensitive to the retrieval results, but the retrieved temperature profiles above 40- 50 km were not so good. Thus MLS temperature products (v2.2) with applying migrating tidal model (Global Scale Wave Model) was referred as the mesospheric temperature field.
- Preliminary correction in observed frequency grids has been introduced. By removing residue of frequency fitting in L1B data, the residue is decreased from 100 kHz to 50 kHz.
- Some line parameters have been updated (seeTable 6).
- Bugs in frequency grids around $O^{17}OO$ (Band B) and ^{18}OOO (Band C) have been fixed. This update reduces systematic error above 50km.

Table 6 updated line parameters

Parameters	L2 v1.3	v2.0	Reference
O_3			
- γ_0 **(MHz/hPa)**	624371.112	624371.223	Ozeki private communication (preliminary results)
- n_γ	2.258	2.3078	HITRAN2008
	0.77	0.78	HITRAN2008
$H^{35}Cl$			
- **Line position (MHz)**	625901.603	625901.6584	Colmont et al., 2005
	625918.756	625918.6975	
	625932.007	625932.0081	
- γ_0 **(MHz/hPa)**	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
$H^{37}Cl$			
- **Line position (MHz)**	624964.374	624964.3694	Colmont et al., 2005
	624977.821	624977.8013	
	624988.334	624988.2821	
- γ_0 **(MHz/hPa)**	2.57	2.541	MLS Forward model ATBD (v1.0)
- n_γ	0.73	0.723	MLS Forward model ATBD (v1.0)
ClO			
- **Line position (MHz)**	649445.040	649445.250	Oh and Cohen, 1994
	649451.170	649451.072	
^{18}OOO			
- **Line position (MHz)**	649137.611	649137.132	Ozeki private communication (preliminary results)
	649137.611	649137.132	
	649149.603	649152.038	
	649152.601	649152.038	